2-(Methylsulfanyl)quinoxaline 21948-73-2 | DTXSID00325902

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	1.14	0.85	1.12	0.83	1.23	

Model Results

Predicted value: 4.81e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.06e-01

Confidence level: 6.83e-01

Nearest Neighbors from the Training Set

Image not found 1,4-Benzoquinone

Measured: 4.60e-12 Predicted: 5.97e-12